

WHAT IS CLAIMED IS:

1. A method for selecting a best case set of factor levels of a catalyzed chemical reaction, comprising;

5 defining a catalyzed chemical experimental space according to a Latin square strategy; and

effecting a combinatorial high throughput screening (CHTS) method on the catalyzed chemical experimental space to select a best case set of factor levels from the catalyzed experimental space.

10 2. The method of claim 1, wherein the space is defined according to a Graeco-Latin square design.

3. The method of claim 1, wherein the space is defined according to a Hyper-Graeco-Latin square design.

15 4. The method of claim 1, wherein the space is defined according to a Youden Square design.

5. The method of claim 1, wherein the space is defined by (i) identifying candidate factor levels of the space; and (ii) arranging the candidate factor levels into the chemical experimental space according to a Latin square design.

6. The method of claim 1, wherein the space is defined by a Latin square matrix representing t number of factor levels.

20 7. The method of claim 1, wherein the space is defined by a Latin square matrix representing t number of factor levels by: (1) postulating a t x t sized matrix; (2) designating factors with letters of the alphabet; (3) assigning the letters in alphabetical order to a first matrix row of t units; and (4) assigning subsequent alphabetically ordered representative letters to succeeding t number of rows,
25 beginning each row with an alphabetically succeeding letter until the matrix is filled.

8. The method of claim 1, wherein the space is defined according to a Latin square design by generating a plurality of tables of factor levels and merging the tables into a single table.

5 9. The method of claim 1, wherein the space is defined according to a Latin square strategy by generating a plurality of tables of factor levels and merging the tables into a single table by creating a union of tables whenever the tables have factor levels in common.

10 10. The method of claim 1, wherein the space is defined according to a Latin square design by generating a plurality of tables of factor levels and merging the tables into a single table by creating a merger of tables whenever the tables have factor levels in common and folding a smaller table into a larger table of the tables whenever the tables have no factor level in common.

11. The method of claim 1, wherein results of effecting the CHTS method are analyzed by analysis of variance.

15 12. The method of claim 1, wherein results of effecting the CHTS method are analyzed by Percent of Variance Explained.

13. The method of claim 1, wherein results of effecting the CHTS method are analyzed by applying Tukey Simultaneous Tests.

20 14. The method of claim 1, wherein results of effecting the CHTS method are analyzed by determining ratios (t values) of mean values of results and standard error and determining whether differences in the ratios are statistically significantly different to identify leads.

15. The method of claim 1, wherein the experimental space is defined by two or more factors, each having a plurality of possible levels.

25 16. The method of claim 1, wherein the CHTS comprises effecting parallel chemical reactions of an array of reactants defined as the experimental space.

17. The method of claim 1, wherein the CHTS comprises effecting parallel chemical reactions on a micro scale on reactants defined as the experimental space.

5 18. The method of claim 1, wherein the CHTS comprises an iteration of steps of simultaneously reacting a multiplicity of tagged reactants and identifying a multiplicity of tagged products of the reaction and evaluating the identified products after completion of a single or repeated iteration.

19. The method of claim 1, wherein the experimental space factor levels comprise reactants, catalysts and conditions and the CHTS comprises

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10 (A) (a) reacting a reactant selected from the experimental space under a selected set of catalysts or reaction conditions; and (b) evaluating a set of products of the reacting step; and

(B) reiterating step (A) wherein a selected experimental space selected for a step (a) is chosen as a result of an evaluating step (b) of a preceding iteration of step (A).

20 20. The method of claim 19, wherein the evaluating step (b) comprises identifying relationships between factor levels of the candidate chemical reaction space; and determining the chemical experimental space according to a Latin square design for the next iteration.

21. The method of claim 19, comprising reiterating (A) until a best set of factor levels of the chemical experimental space is selected.

22. The method of claim 1, wherein the chemical space includes a catalyst system comprising a Group VIII B metal.

25 23. The method of claim 1, wherein the chemical space includes a catalyst system comprising palladium.

24. The method of claim 1, wherein the chemical space includes a catalyst system comprising a halide composition.

25. The method of claim 1, wherein the chemical space includes an inorganic co-catalyst.

5 26. A system for investigating a catalyzed experimental space, comprising;

a programmed controller that defines a catalyzed chemical experimental space according to a Latin square strategy; and

10 a reactor for effecting a CHTS method on the catalyzed chemical experimental space to produce results.

27. The system of claim 26, wherein the controller is a computer, processor or microprocessor.

15 28. The system of claim 26, further comprising a dispensing assembly to charge factor levels of reactants or catalysts representing the catalyzed chemical experimental space to wells of an array plate for charging to the reactor.

29. The system of claim 29, comprising a programmed controller to define the catalyzed chemical experimental space and to control the assembly to charge factor levels of reactants or catalysts according to the controller defined space.

20 30. The system of claim 26, further comprising a detector to detect results of the CHTS method effected in the reactor.

31. A method, comprising:

selecting a set of reactant factors and their levels and a set of process factors and their levels;



ordering the levels by a Latin square strategy to define an experimental space;

effecting a CHTS method by performing runs of the experimental space in a CHTS system;

5 analyzing data from the runs with graphical and statistical tools to determine a set of factor levels that provides a best result from the experimental space;

determining whether the set of factor levels is a significant set by examination by a statistical technique comprising Percent of Variance Explained and Tukey Simultaneous Test; and

10 reiterating the process if values of the best factor levels are not significant.

32. The method of claim 31, wherein the CHTS method is effected by introducing chemical combinations representing levels into a formulation system comprising a geometrical array and processing the array of chemical combinations into products.

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